Phenol, 2,6-bis[[3-(1,1-dimethylethyl)-2-hydroxy-5-methylp

Other names: Antioxidant 80
Mesitol, «alpha»2,«alpha»6-bis(5-tert-butyl-6-hydroxy-m-tolyl)-
p-Cresol, 2,6-bis(2-hydroxy-3-tert-butyl-5-methylbenzyl)
2,6-bis[[3-(tert-butyl)-2-hydroxy-5-tolyl]methyl]-4-methylphenol

Inchi: InChI=1S/C31H40O3/c1-18-10-21(16-23-12-19(2)14-25(28(23)33)30(4,5)6)27(32)22(11-

InchiKey: LKALLEFLBKHPTQ-UHFFFAOYSA-N

Formula: C31H40O3

SMILES: Cc1cc(Cc2cc(C)cc(C(C)(C)C)c2O)c(O)c(Cc2cc(C)cc(C(C)(C)C)c2O)c1

Mol. weight [g/mol]: 460.65

CAS: 90-68-6

Physical Properties

Property code	Value	Unit	Source
gf	31.41	kJ/mol	Joback Method
hf	-591.83	kJ/mol	Joback Method
hfus	58.36	kJ/mol	Joback Method
hvap	131.85	kJ/mol	Joback Method
log10ws	-8.37		Crippen Method
logp	7.505		Crippen Method
mcvol	393.980	ml/mol	McGowan Method
pc	1270.06	kPa	Joback Method
tb	1254.00	K	Joback Method
tc	1535.50	K	Joback Method
tf	933.51	K	Joback Method
vc	1.323	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1487.45	J/mol×K	1254.00	Joback Method
cpg	1719.11	J/mol×K	1488.58	Joback Method
cpg	1664.00	J/mol×K	1441.67	Joback Method
cpg	1613.79	J/mol×K	1394.75	Joback Method
cpg	1567.97	J/mol×K	1347.83	Joback Method

cpg	1526.03	J/mol×K	1300.92	Joback Method
cpg	1779.65	J/mol×K	1535.50	Joback Method
dvisc	1.3452054e-10	Pa×s	1254.00	Joback Method
dvisc	1.9903093e-10	Pa×s	1200.59	Joback Method
dvisc	3.0541901e-10	Pa×s	1147.17	Joback Method
dvisc	4.8869319e-10	Pa×s	1093.76	Joback Method
dvisc	8.2061447e-10	Pa×s	1040.34	Joback Method
dvisc	1.4574994e-09	Pa×s	986.92	Joback Method
dvisc	2.7645638e-09	Pa×s	933.51	Joback Method

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C90686&Units=SI

Legend

cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
gf: Standard Gibbs free energy of formation
hf: Enthalpy of formation at standard conditions
hfus: Enthalpy of fusion at standard conditions
hvap: Enthalpy of vaporization at standard conditions
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
pc: Critical Pressure
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume

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